Estimation of Thermophysical Pure Component Properties from Molecular Structure
Structure Editor, Group Assignment, Structure Database

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For the synthesis, design and simulation of chemical processes, reliable knowledge of thermophysical pure component and mixture properties is of great importance. Often these data are not available or are of questionable quality. That is the reason why besides large factual databases like the Dortmund Data Bank (DDB), also estimation methods are often needed.

For this reason the authors developed a program system for the estimation of a variety of pure component properties covering

- P-v-T data like saturated vapor pressures, normal boiling points, critical temperatures, pressures, volumes, densities of liquid and vapors, and virial coefficients
- Transport properties like viscosities of liquids and vapors and thermal conductivities
- Thermal properties like heat capacities of liquids and gases, heats of fusion, vaprorization, formation, and combustion
- Others properties like water solubilities, topological indices, etc.

The program system contains a Windows-based structure editor (ARTIST) for molecules and a database system (ChemDB) for storing and retrieving the molecular structures as connection tables.

The estimation procedures have been implemented around an automatic group assignment algorithm which allows the examination of the constitition of a molecular structure by a table of functional group descriptions. The list of group descriptions are prepared for the single models and can then be used for all structures either drawn with the structure editor or retrieved from the structure database. The algorithm retrieves the list of the groups a structure is comprised of and gives also some additional information like rings, chains, aromaticity, ortho/meta/para positions, longest path through the structure, etc.

The list of models currently implemented comprises

- Critical data by Joback, Gani/Constantinou, Wen/Qiang, Ambrose, Somayajulu, Marrero/Pardillo, Lydersen, Daubert, Tu
- Normal boiling point by Stein/Brown, Joback, Ambrose, Lydersen, Devotta/Rao and a new method from the authors
- Heat capacities by Benson, Seaton, Ruzicka/Domalski, Garvin, Luria/Benson
- Thermal Conductivity by Nagvekar/Daubert, Sastri/Rai, Lakshmi
- Heat of vaporization by Basarova/Svoboda

This work has been developed in close cooperation with a pure component properties database project which has the aim to cover all worldwide available experimental data. This database contains currently 130,000 data sets with 850,000 data points and is increasing by approx. 10,000 data sets per year. The database and the described estimation program are the base for obtaining thermophysical data for the usage in process design without expensive measurements.

Besides the lecture, program demonstrations are also available on request.